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Best Available Copy

TITLE

A QUICK AND SIMPLE DATABASE FOR COMPARING TOXIN SEQUENCE DATA

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Running Title: A Quick and Simple Database

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ABSTRACT

F. W. SEXTON. A quick and simple database for comparing toxin sequence data. *Toxicon* ..,, 19.. __We describe a method for using two computer programs, a word processor and a search program, to create a workable, inexpensive database. With these programs, we created databases for comparing toxin sequence data, storing lists of publications and producing a list of technical publications. These databases were easily created and are "user friendly".



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There is a need for databases in any laboratory. In our laboratory, we needed ways of storing toxin sequences data, lists of publications and technical information. We use Apple Macintosh® computers with hard disk drives. To create the databases, we used the programs, Microsoft Word, Version 4.0 (Microsoft Corporation Redmond, Washington; and Microlytics GOfer (Microlytics, Inc., Pittsford, New York). Microsoft Word is a word-processing program; GOfer is a "desk accessory" that can be used to search files at any time just by choosing the program from the "APPLE" desk accessories menu. GOfer must first be installed into the computer's operating system according to the manufacturer's instructions.

Information to be stored is first entered into the computer by using Microsoft Word. Table I shows an example of the format of entries, in this case, toxin sequence data. Once data are entered, GOfer is chosen from the list of desk accessories under the Apple icon on the far left of the Apple screen. When the program responds with a request blank for a search (Table I), information is entered as requested, and the program searches the computer files. Finds are displayed on the screen and can be printed as a report.

Figure 1 shows a report generated from a request for components of toxins that are common to several toxins. Figure 2 is a similar report, but is a listing of all publications, in the database, that deal with the snake Notechis.

The ability to search through any type of format, plus the ability to generate a report, makes the Microsoft Word/GOfer system efficient and desirable. The variety of information stored and its format are unlimited. In addition to Word, there are several other word processing programs available for the Macintosh that are supported by GOfer. Such programs are listed in its on-screen support file.

TABLE I

A. Procedure for entering data:

1. For toxin Sequences;

- a. 1st line-Number. Organism Name Type of Toxin
- b. 2nd line-Sequence

Example:

215 NOTECHIS scutatus scutatus Notexin
GENGPY-CRNIKKKCLRFVCDVCDVEAAFCFAKAPYMNANWNIDTKKRCQ

2. For publication references:

- a. 1st line-Number Title
- b. 2nd line-Author(s)
- c. 3rd line-Publication, year, volume, number, page numbers

Examples:

6. Molecular Mimicry and Myasthenia Gravis

Schwimmbeck. PL; Dyrberg, T; Drachman, DB; Oldstone,
MBA.

BOOK: Molecular Mimicry, Myasthenia Gravis, and
Herpes Simplex pg 1174-1180

8. Proteolytic fragments of the nicotinic acetylcholine receptor identified by mass spectrometry: Implications for receptor topography.

Moore, CR; Yates, Jr III; Griffin, PR; Shabanowitz, J;
Martino, PA; Hunt, DF; Cafiso, DS
Biochemistry, 1989, vol 28, pg 9184-9191

B. Search Steps

1. Toxin search

- A. Open the file you want searched.
- B. Call GOfer from Apple icon
- C. Tell GOFER What, Where, and How, then click on the GOfer Box.
- D. After the search is done, pull down the GOfe Menu, select:
Export
Current Found File
Each Find, enter "1" in 1st box.
Enter number in second box if needed
Fill in name of Export program (We use PRINT).
- E. Open "PRINT", print report.

By using a monospaced font (i.e. Courier), all sequences will have letters spaced equal distance apart, prior to printing the report (if desired) all extraneous material may be deleted, thus making for easier comparisons when the report of a search is made.

The reports, in Figures 1 & 2, show some of the types of information and format that may be used with these two programs.

FIGURE CAPTION PAGE

Figure 1. GOfer report on a search for four specific amino acids from the snake toxin sequence data base.

Figure 2. GOfer report on a search for a specific toxin name in the publications data base.

What: KKQW
Exactness: Ignore Case/WildCard
Files Searched: 1
Bytes Searched: 29134
Found Files: 1
Total Finds: 5
Exporting... each find - 1 + 0 lines

File: TOXINS:TOXINS
Kind: Microsoft Word document
Bytes: 29134
Finds: 5

..... Found text starting with find # 1 , lines 18 to 19
5. HEMACHATUS hemachatus Toxin - IV
LECHNQSSQTPTTQTOP-GETNOCYKQWSDHRGSRTERGCGCPTVK-PGIXLKCUITDRCNK

..... Found text starting with find # 2 , lines 26 to 27
9. NAJA melanoleuca Toxin d
MECHNQSSQPPTTKTOP-GETNOCYKQWSDHRGTIIIEPGCGCPSVK-KGVKINCCTTDRCNN

..... Found text starting with find # 3 , lines 30 to 31
11. NAJA haje haje CM-10a
MICHNQSSQPPTIKTOP-GETNOCYKQWSDHRGTIIIEPGCGCPSVK-KGVGIYCCXTDKCHN

..... Found text starting with find # 4 , lines 62 to 63
27. NAJA haje annulifera CM-10
MICYKQSSLGFPITTVCP-GETNOCYKQWSDHRGTIIIEPGCGCPSVK-KGIEINCCTTDRCNN

..... Found text starting with find # 5 , lines 64 to 65
29. NAJA haje annulifera CM-12
MICYKQSSLGFPITTVCP-GETNOCYKQWSDHRGTIIIEPGCGCPSVK-KGIEINCCTTDRCNN

Figure 1

What: Notechis
Exactness: Ignore Case/WildCard
Files Searched: 1
Bytes Searched: 68096
Found Files: 1
Total Finds: 4
Exporting... each find - 1 + 2 lines

.....
File: Pub I:Pub Ref 1
Kind: Microsoft Word document
Bytes: 68096
Finds: 4
.....

..... Found text starting with find # 1 , lines 441 to 444
107. Purification of a presynaptic neurotoxin from the venom of the
Australian tiger snake *Notechis scutatus scutatus*
Karlsson, E; Eaker, D; Ryden, L
Toxicon, 1972, vol 10, pg 405-413

..... Found text starting with find # 2 , lines 555 to 558
137. Amino acid sequence of a presynaptic neurotoxin from the
venom of *Notechis scutatus scutatus* (Australian tiger snake)
Halpert, J; Eaker, D
Jour Biological Chemistry, 1975, vol 230, #
17, pg 6990-6997

..... Found text starting with find # 3 , lines 601 to 604
148. The mass of venom injected by two Elapidae: the taipan
(*Oxyuranus scutellatus*) and the Australian tiger snake
(*Notechis scutatus*)
Morrison, JJ; Pearn, JH; Coulter, AR
Book: 1982, pg 739-746

..... Found text starting with find # 4 , lines 1099 to 1102
281. Variation in venom proteins from isolated populations of tiger
snakes (*Notechis ater niger*, *N. scutatus*) in southern Australia
Williams, V; White, J; Schwaner, TD; Sparrow, A
Toxicon, 1988, vol 26, # 11, pg 1067-1075

Figure 2